Evolution of Dendritic Extended 3D Patterns during Directional Solidification: Microgravity Experiments in DECLIC-DSI onboard ISS and Phase-field Modeling

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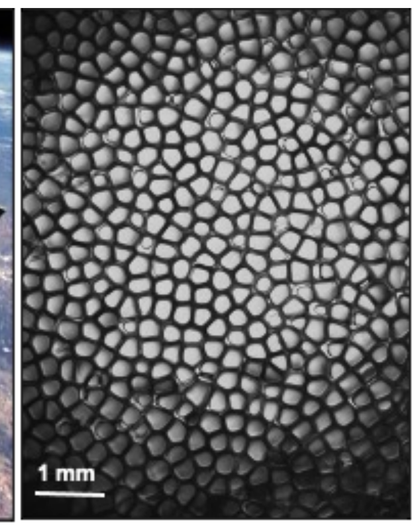
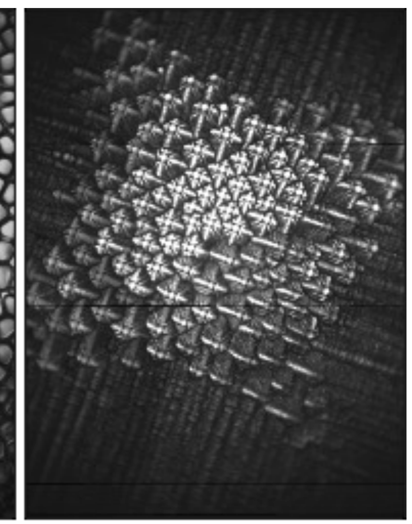
Outline

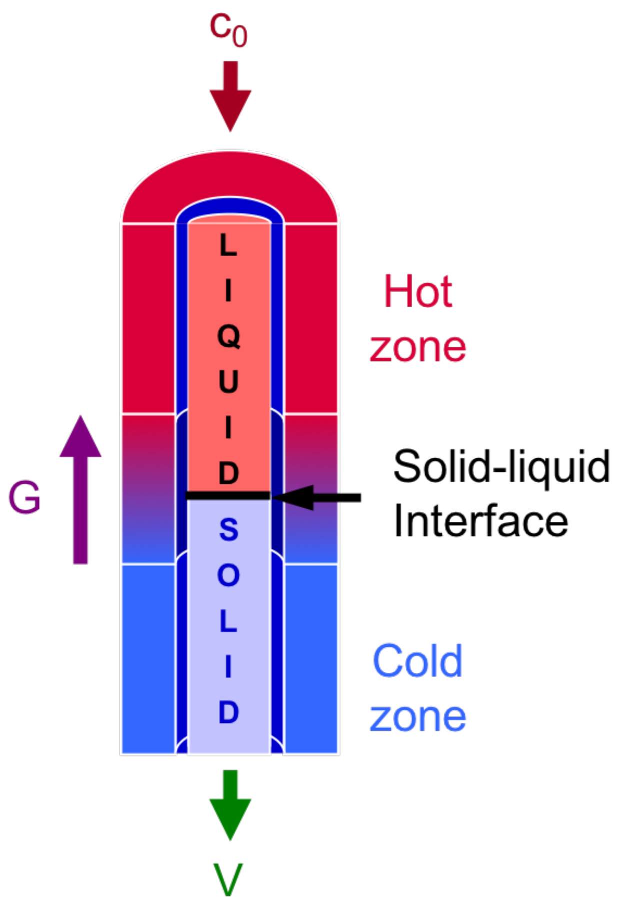
- Microgravity experiment: DEvice for the study of Critical LIquids and Crystallization - Directional Solidification Insert (DECLIC-DSI)
- Phase-field modeling
- DSI-R Campaign
  - ➢ Transient recoil and morphological instability
  - ➢ Dendrite tip radius measurements (using interferometry)
  - ➢ Curvature effects
- Summary and outlook

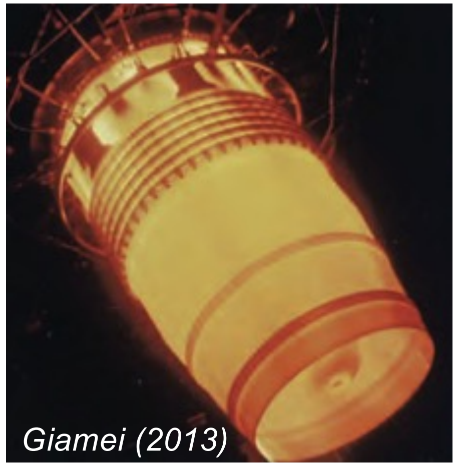


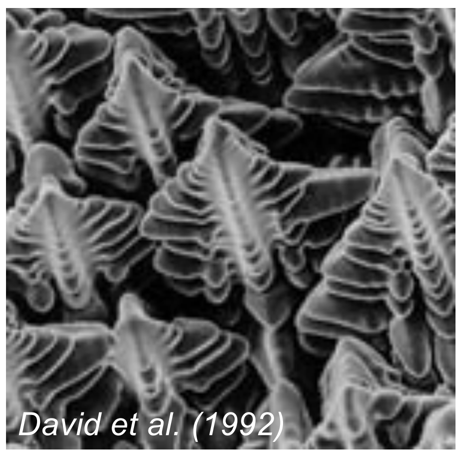


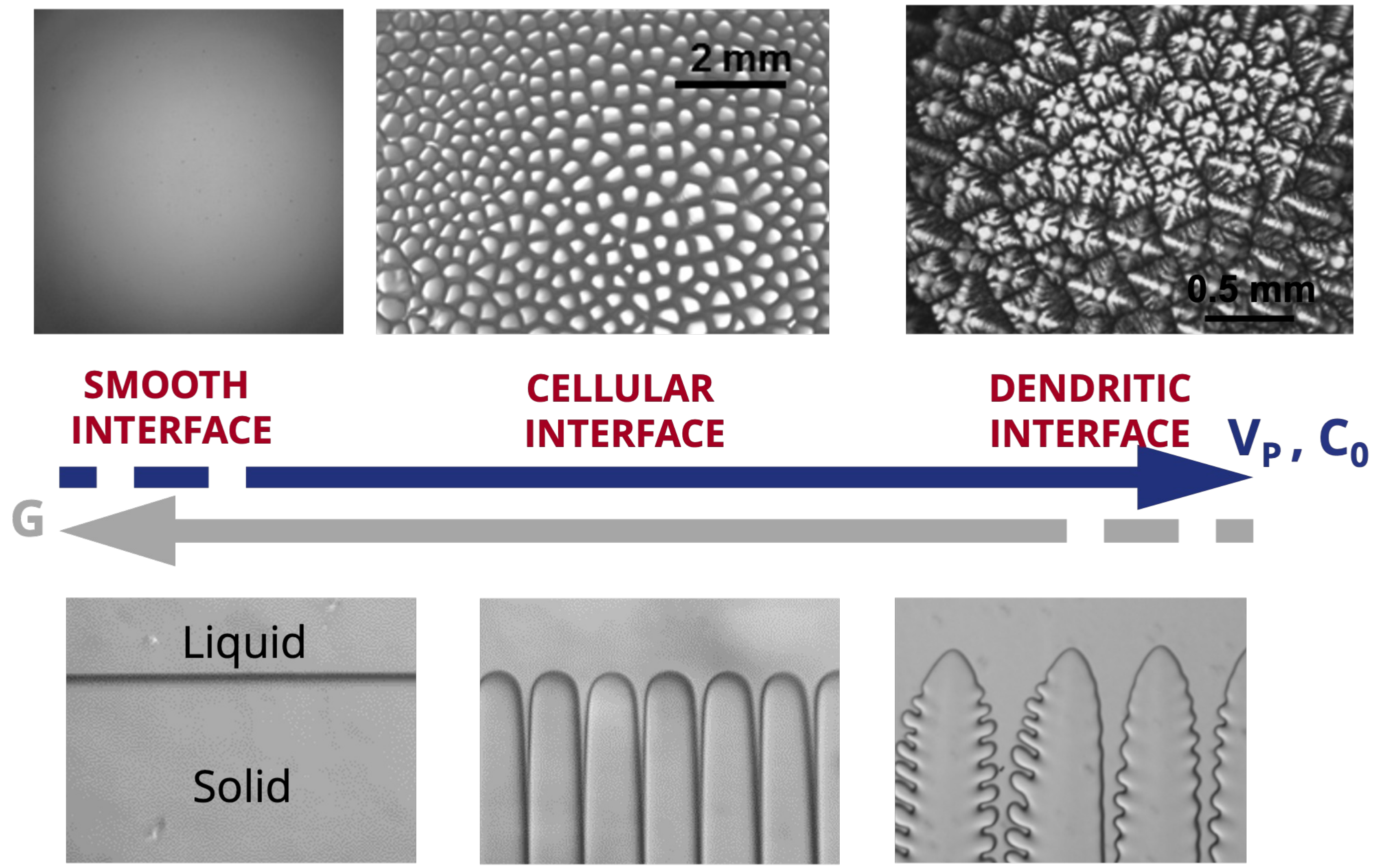
Directional solidification

- Microstructure formation under well-controlled growth conditions during directional solidification: alloy (solute) concentration C_0, a constant pulling rate V_p, and a thermal gradient G.



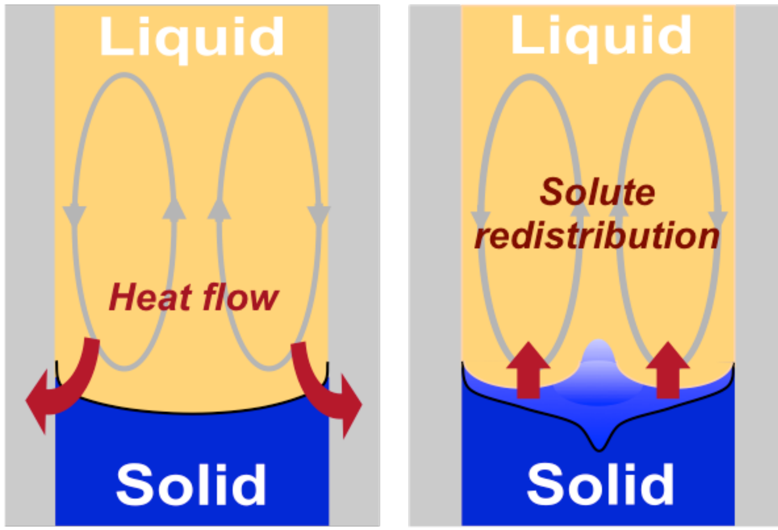

Giamei (2013)


David et al. (1992)

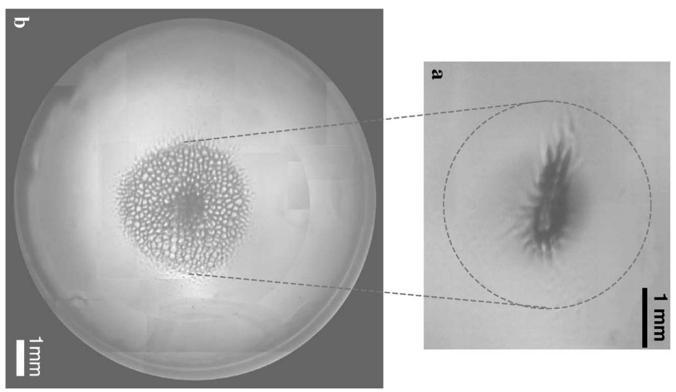


Microgravity experiments

Gravity-induced convection

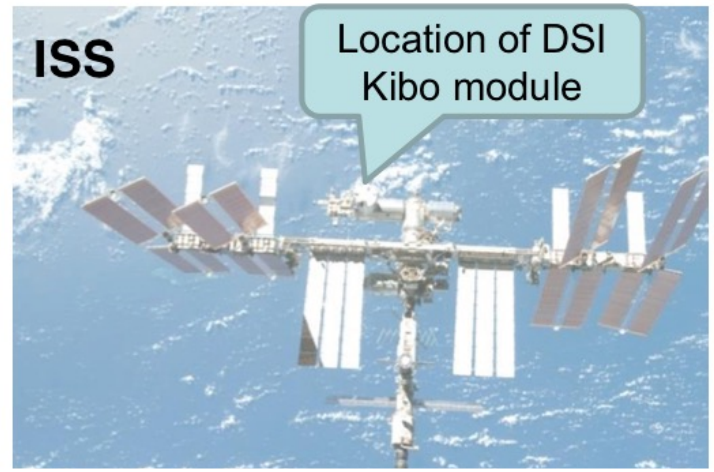


Microstructure heterogeneities



Jamgotchian et al., PRL (2001)

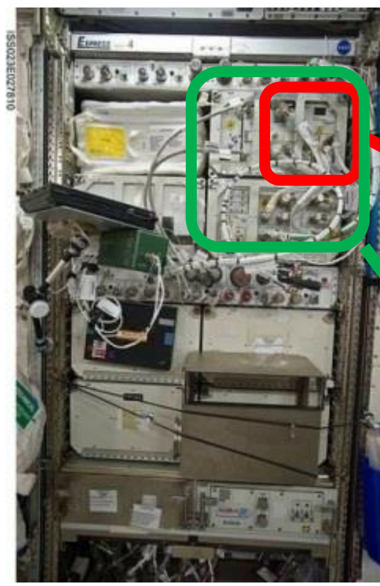
Microgravity experiment



Two campaigns:

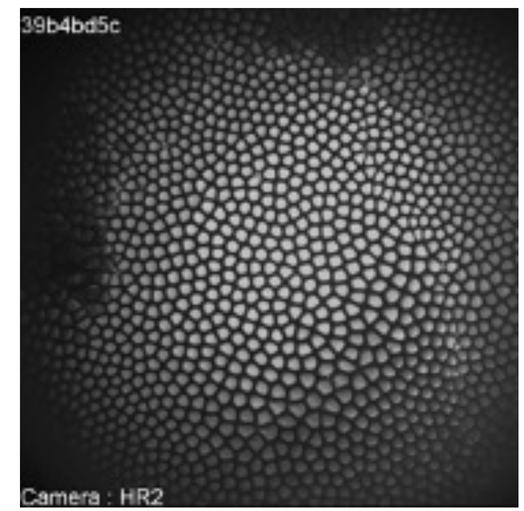
1) Microgravity experiments from **2009-2011** dedicated to cellular regime (**DSI**).

2) Microgravity experiments from **2017-2018** dedicated to dendritic regime (**DSI-R**).



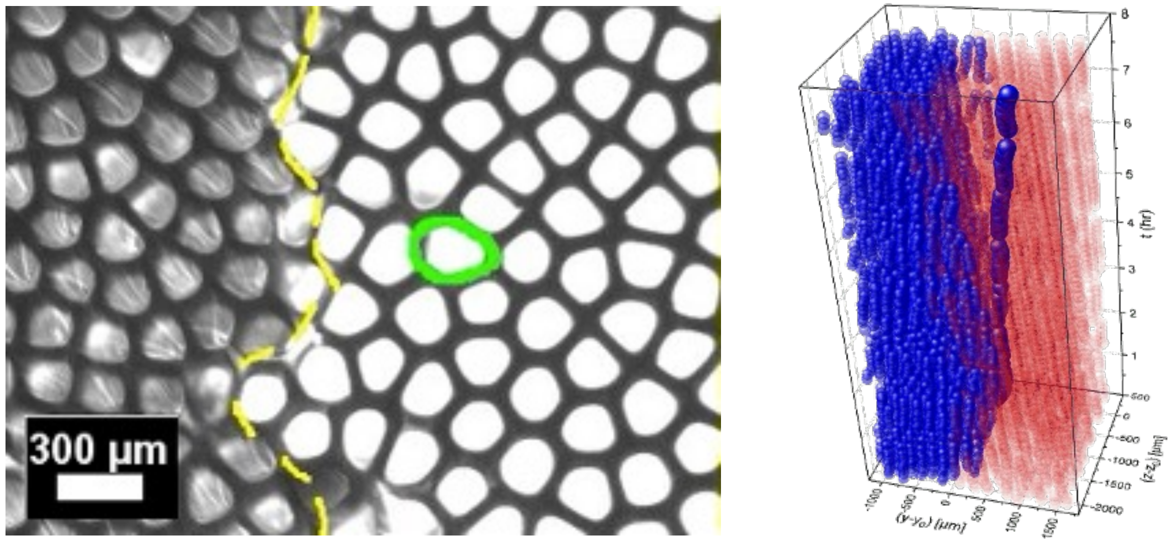
DSI (**D**irectional **S**olidification **I**nsert)

DECLIC

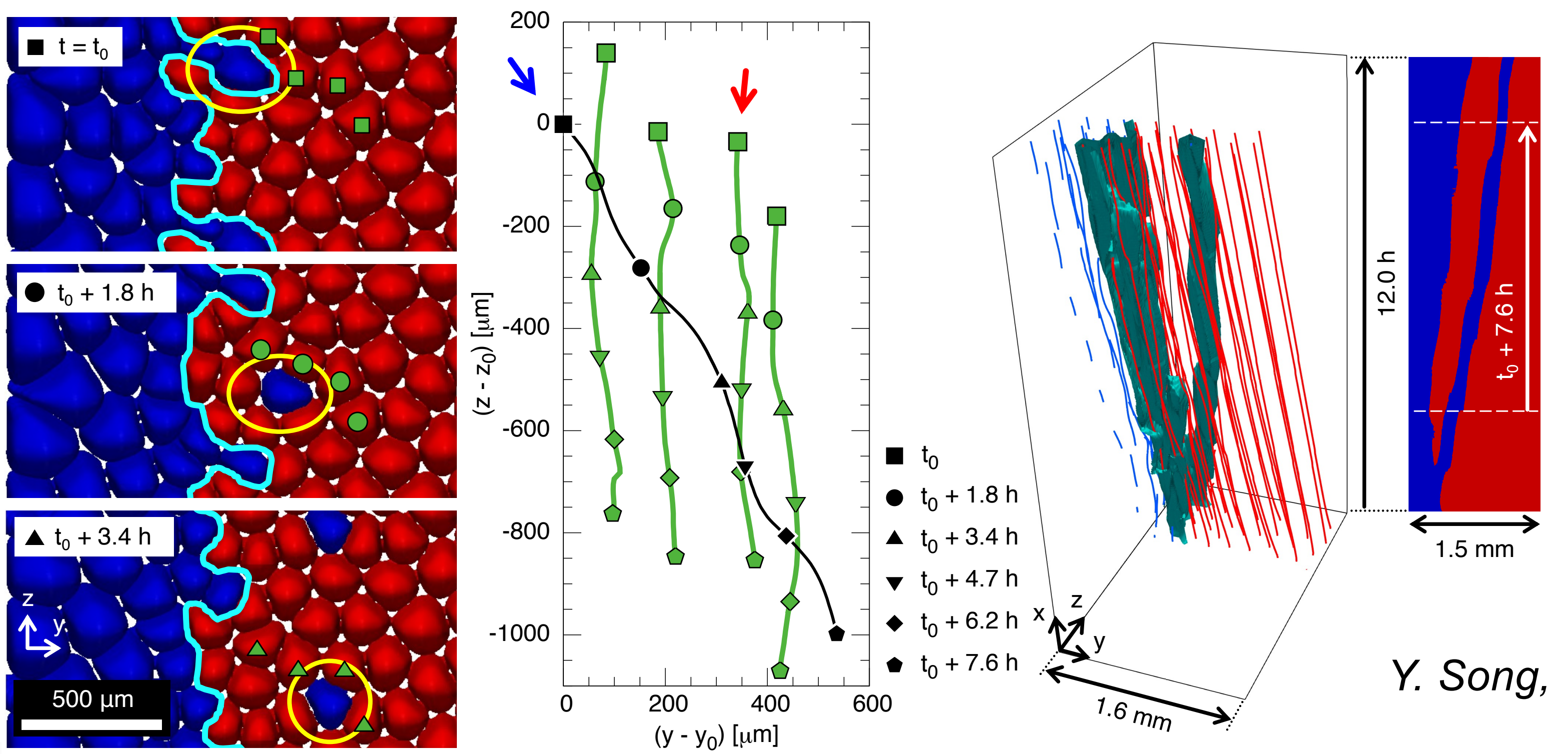


Effects of grain boundary – A combined experimental and PF study

Experiment



Simulation



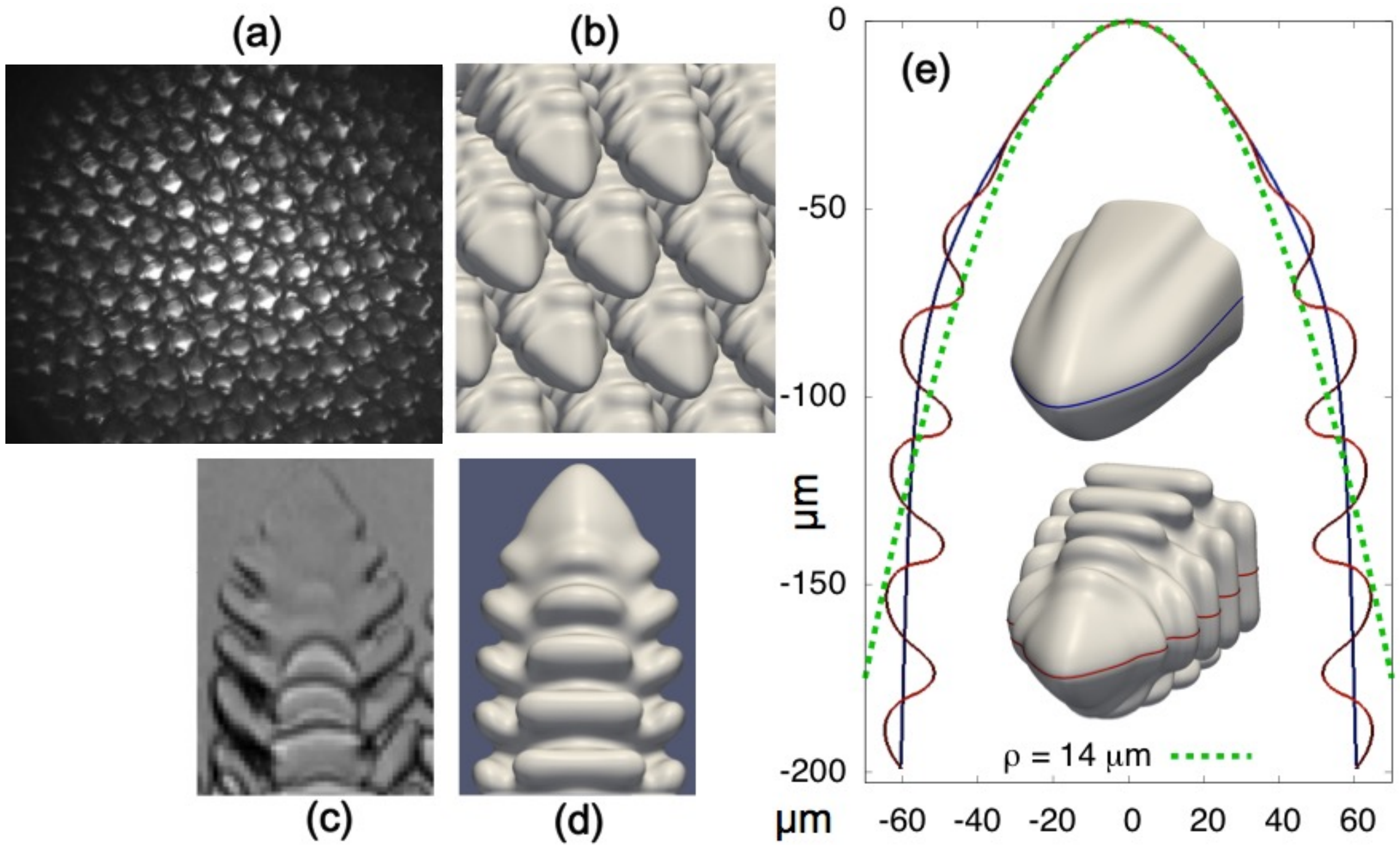
- Individual cells from one grain can invade a nearby grain of different misorientation, causing grains to interpenetrate and grain boundaries to adopt highly convoluted shapes.

- Agreement in the drifting dynamics of solitary cell between phase-field simulations and experiment (DSI).

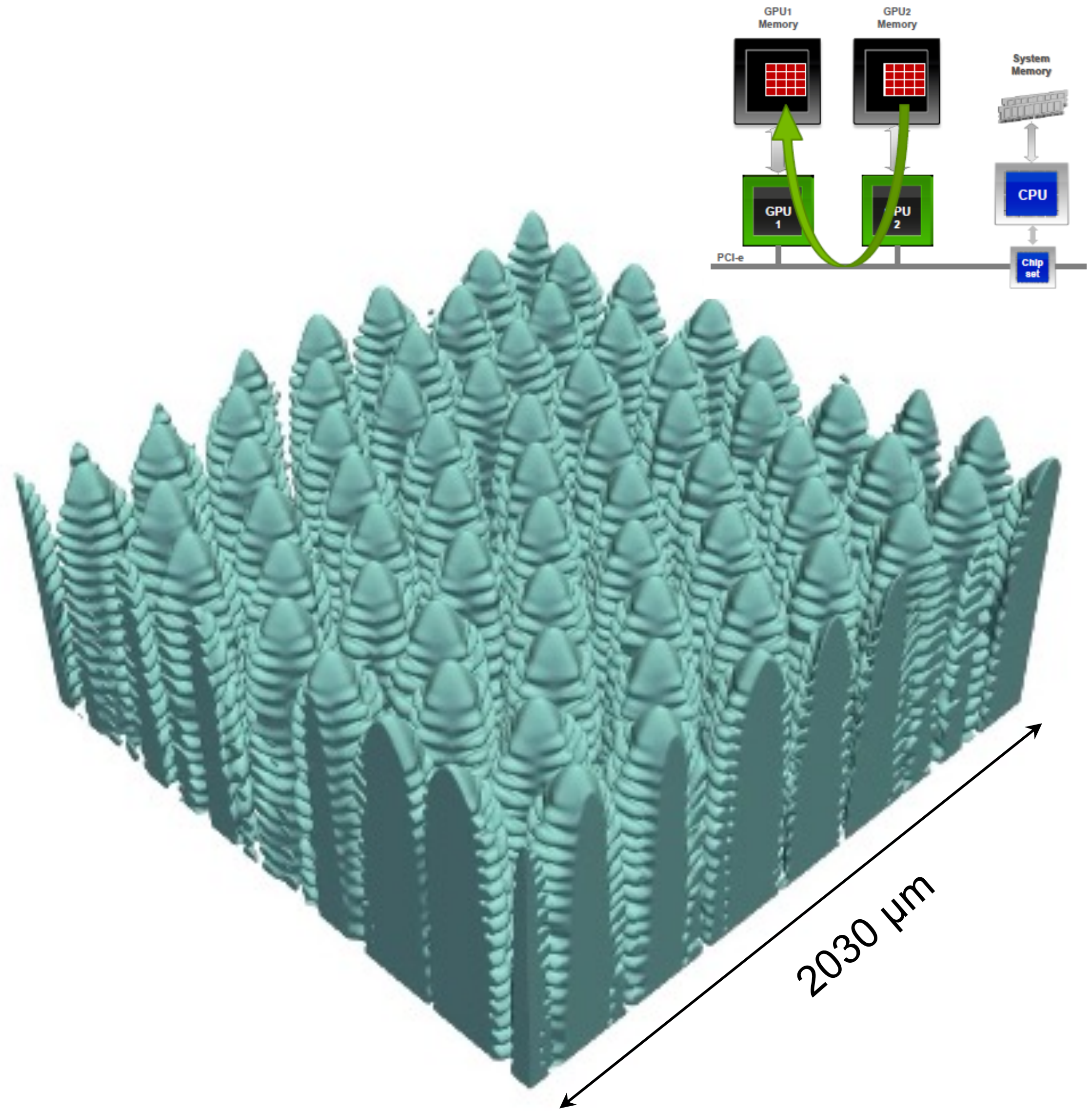
Y. Song, F.L. Mota, D. Tourret, K. Ji, B. Billia, R. Trivedi, N. Bergeon, A. Karma, Nat. Commun., in press

DSI-R Campaign: Increased alloy concentration

- Increase of concentration: dendrites at lower pulling rates
- Study of the formation of dendritic patterns

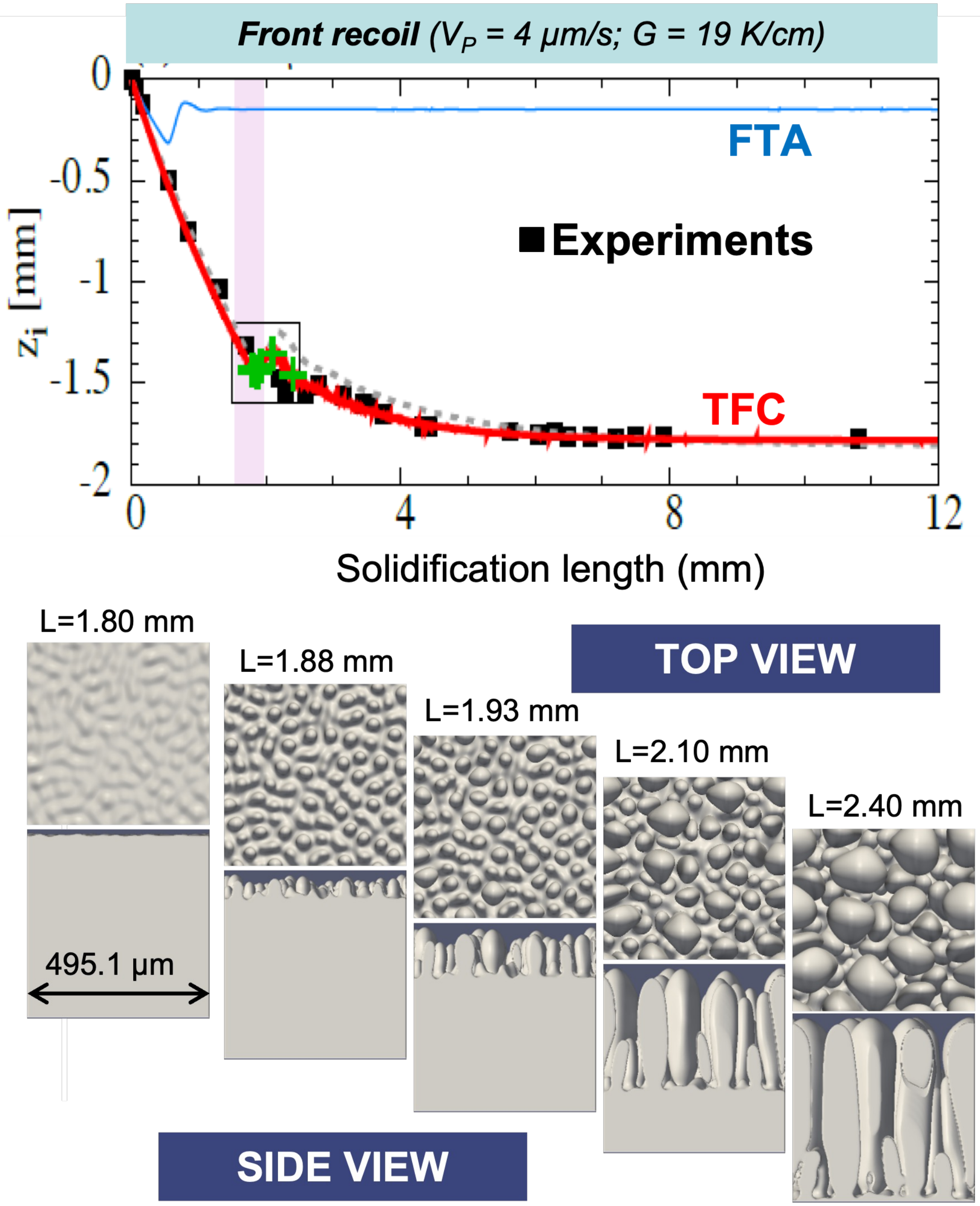


(a) **SCN-0.46wt%** camphor alloy, V_P = 1.5 μm/s, G = 12 K/cm. (b-e) Preliminary results for **SCN-0.5wt%** camphor alloy (V_P = 10 μm/s, G = 23 K/cm): (b) phase-field simulations of dendritic array; (c-d)



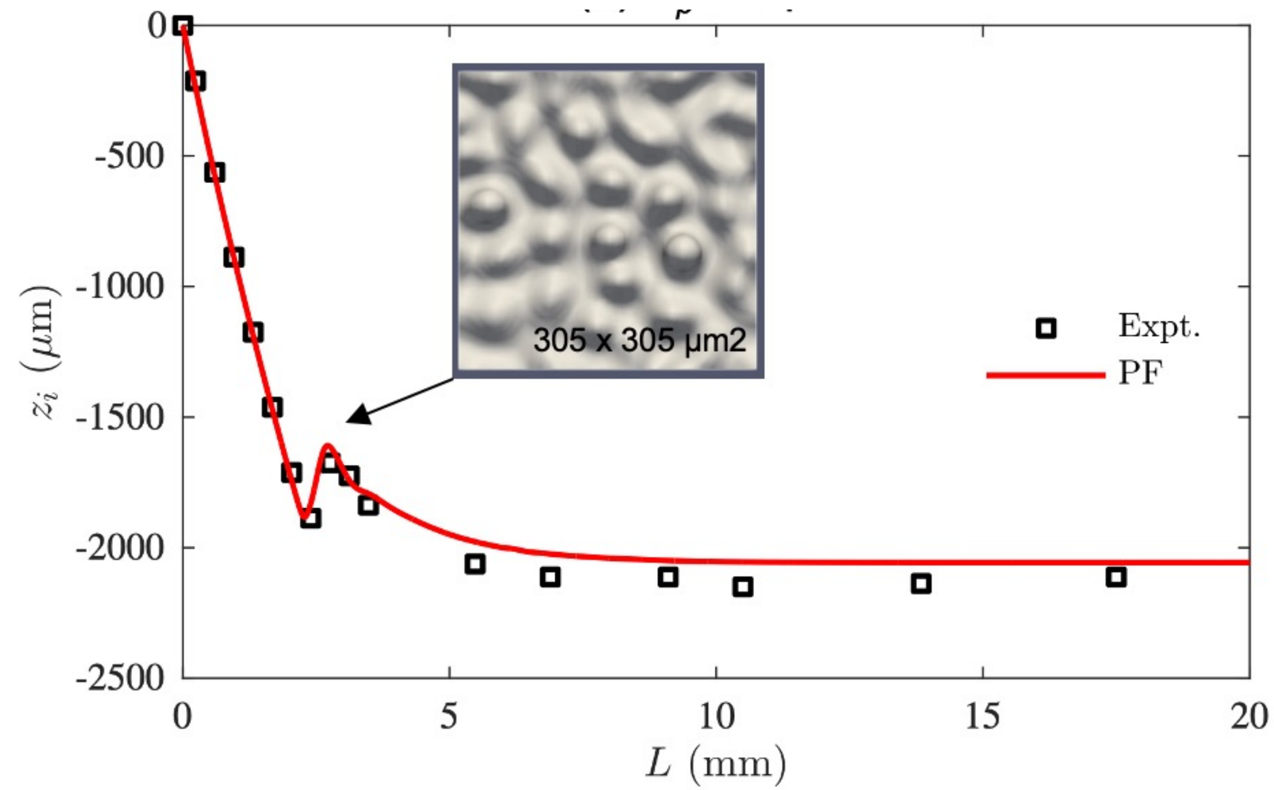
G = 12 K/cm and C_0 = 0.46wt% at V = 1.5–3 µm/s

Solid-liquid interface recoil



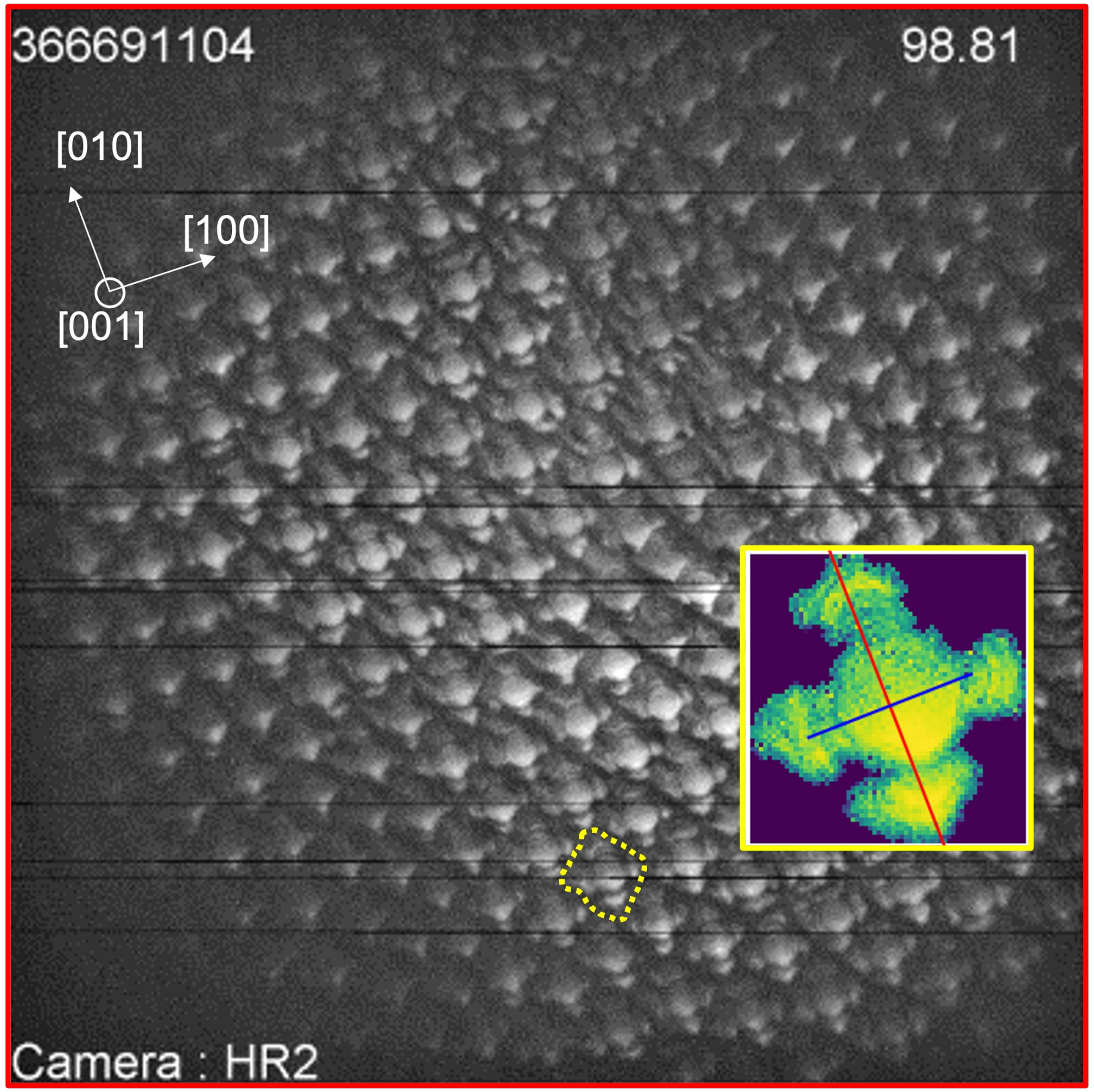
Song et al. Acta Mater (2017)

DSI-R: V = 3 µm/s G = 12 K/cm

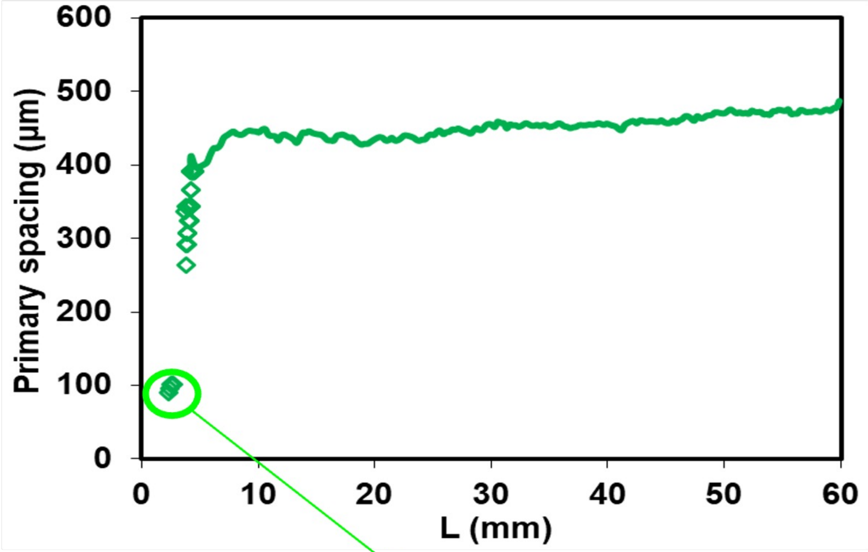


- The interface recoil in the phase-field simulation with latent heat diffusion agrees well to experiment.

Morphological instability

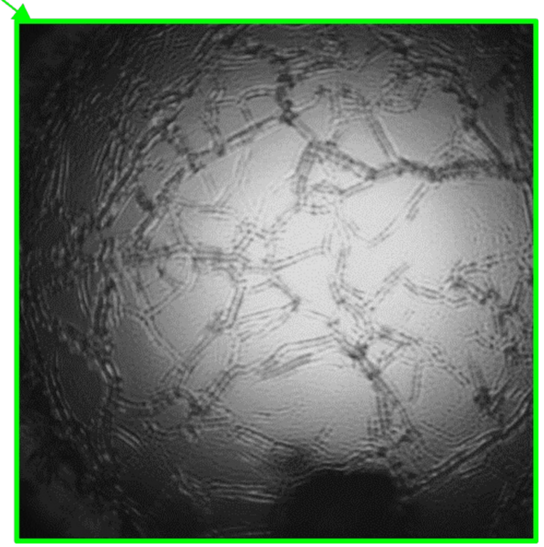


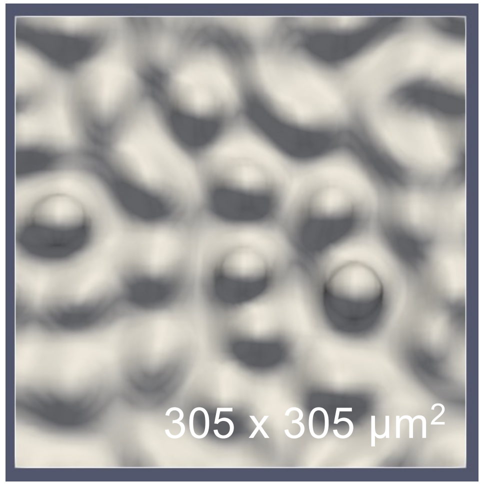
V = 3 μm/s G = 12 K/cm



L = 2.4 mm

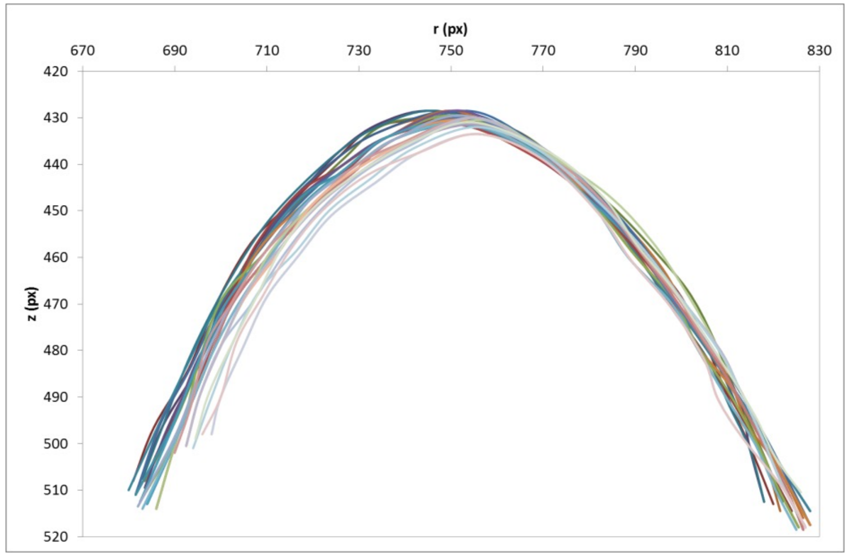
$\lambda_i = 91 \pm 10$ μm



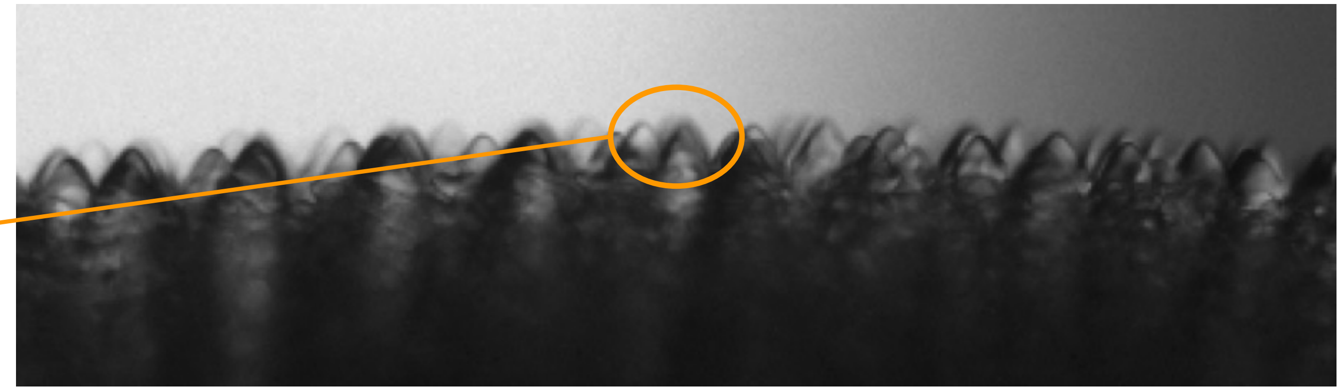


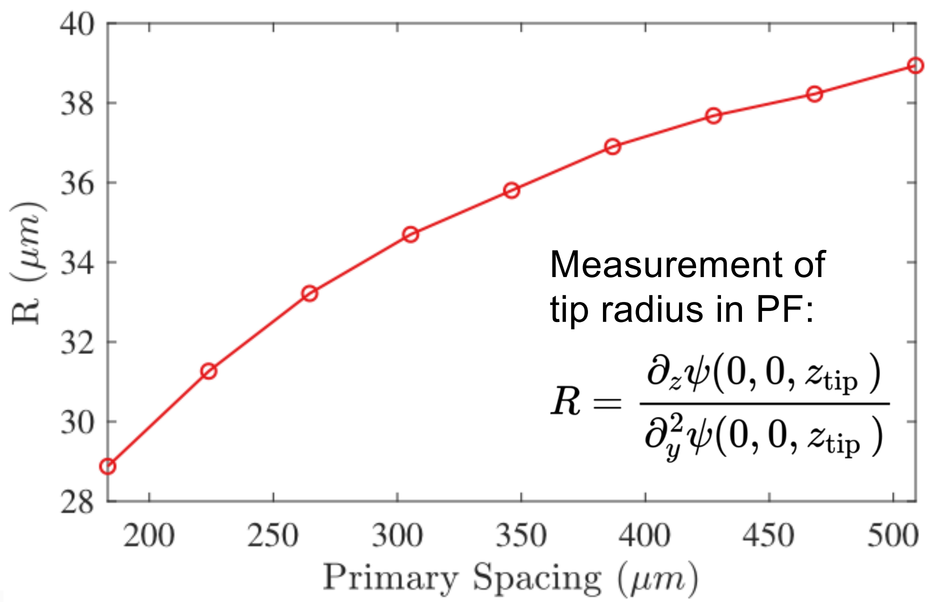
Initial λ ~ **64 μm** in phase-field simulation

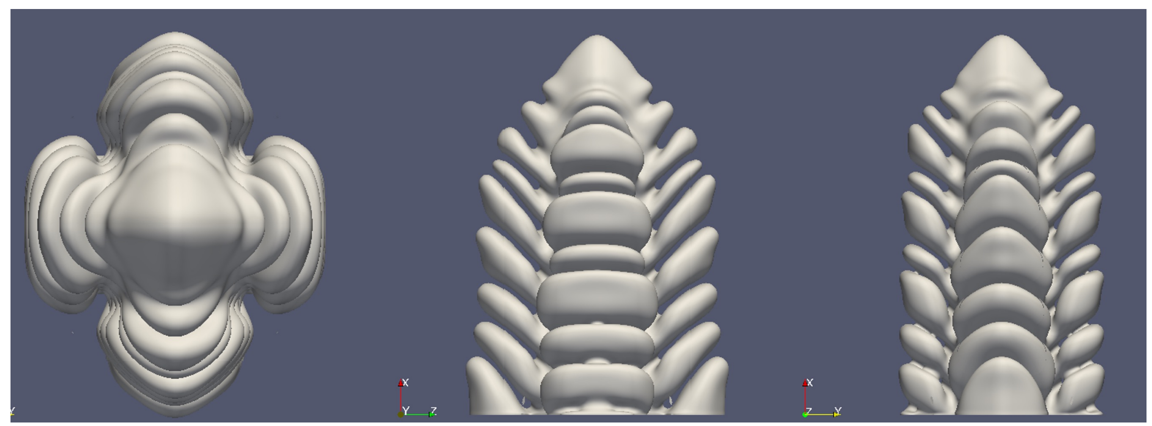
Tip radius measurement



- The tip radius obtained in the PF simulation with (about **39 μm**) agrees well to the experiment measurement of **39 μm**.

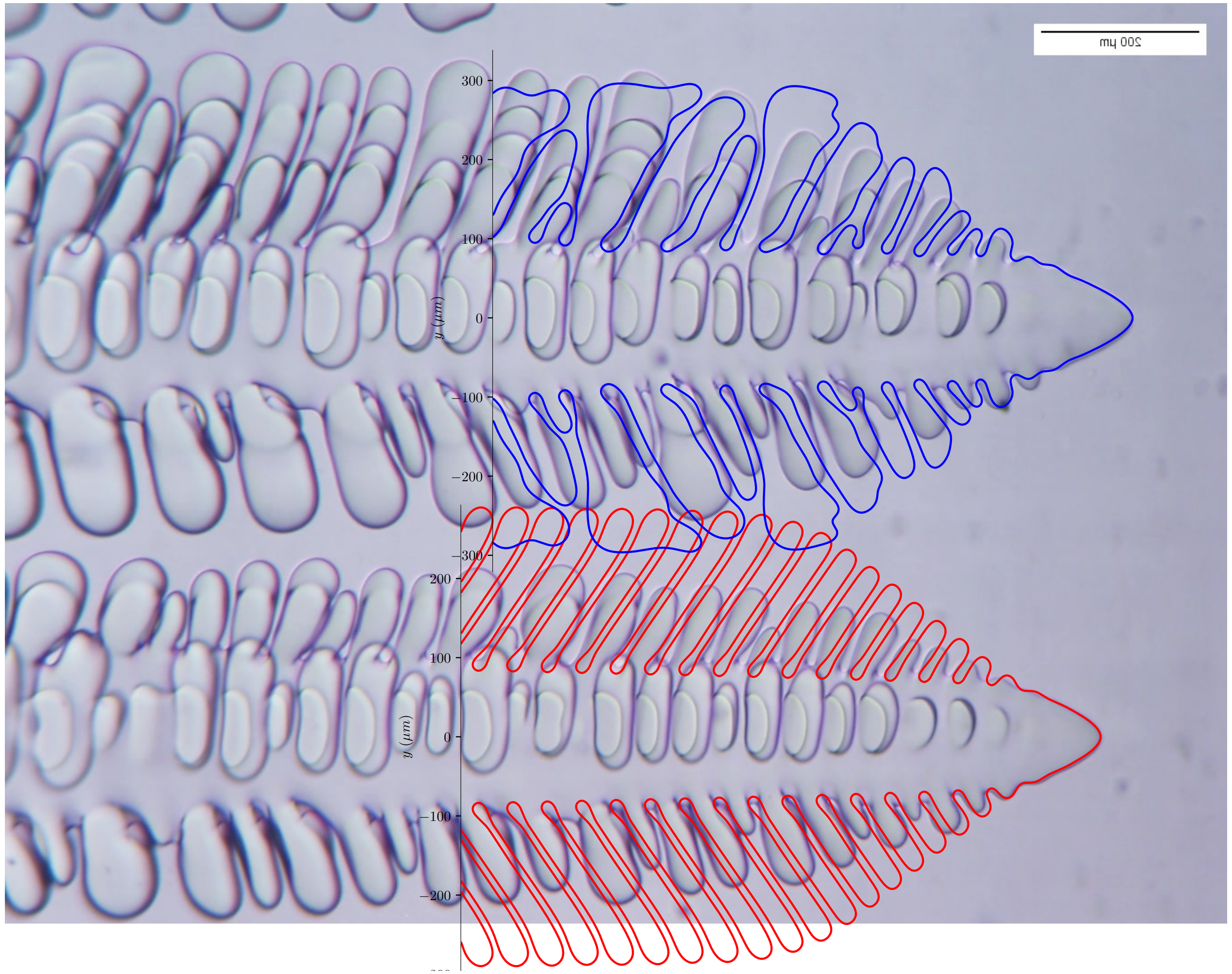






Growth condition: G = 12.5 K/cm and C0 = 0.46wt% at V = 1.5 μm/s

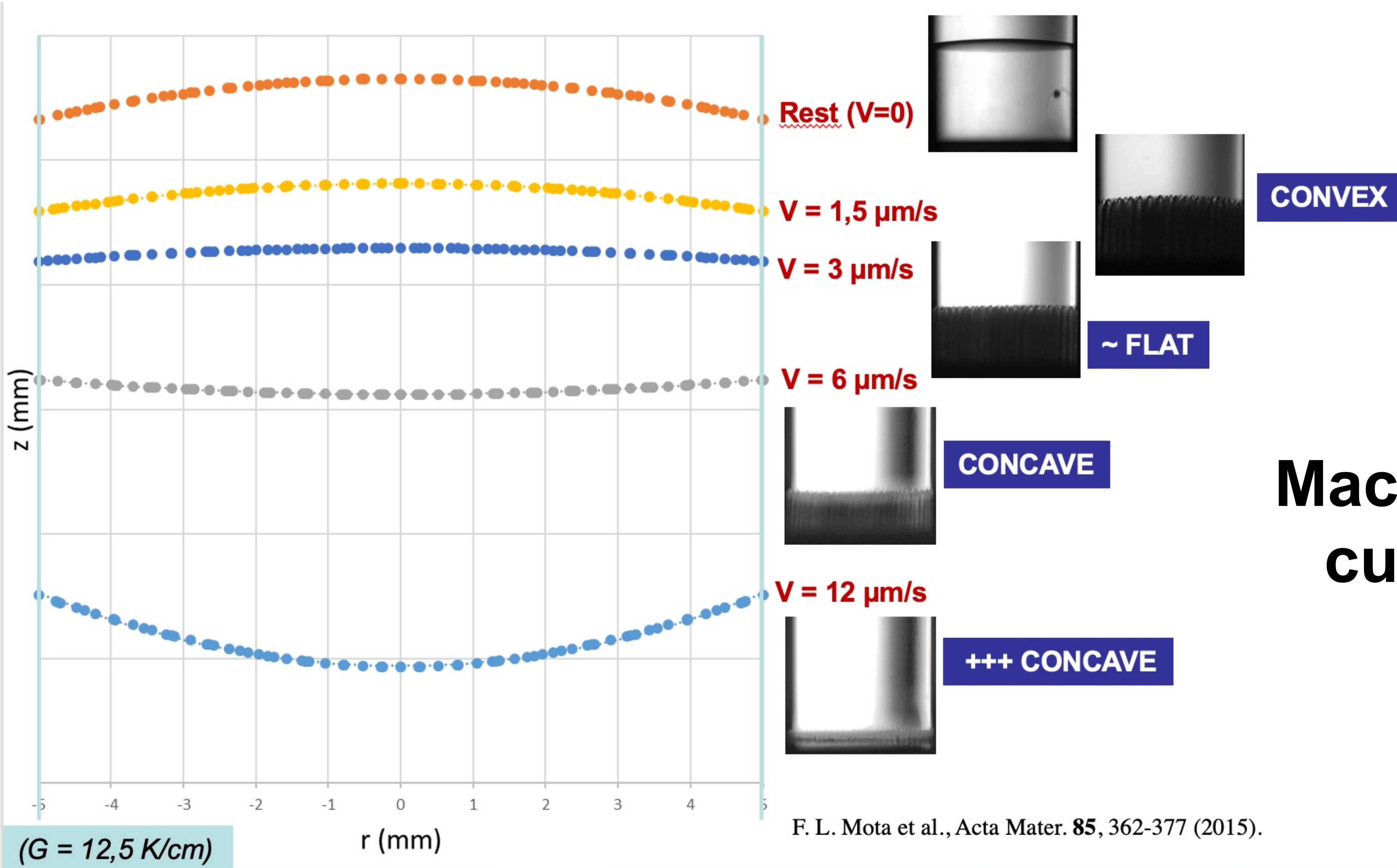
Comparison between PF simulation and experiment



- The PF simulation can quantitatively model a dendrite tip, as validated by thin-sample experiment on the ground.
- The upper limit of primary spacing in the PF simulation is lower than experiments (a separate problem).
- Simulations with the oscillation of temperature around the tip. Promote sidebranching.

$$T(x) = G(x - V_p t) + A\cos(\omega t) e^{-\frac{|\vec{r}-\vec{r}_{tip}|^2}{b^2}}$$

Ground-based experiment: G = 12 K/cm and C_0 = 0.46wt% at V = 6 μm/s



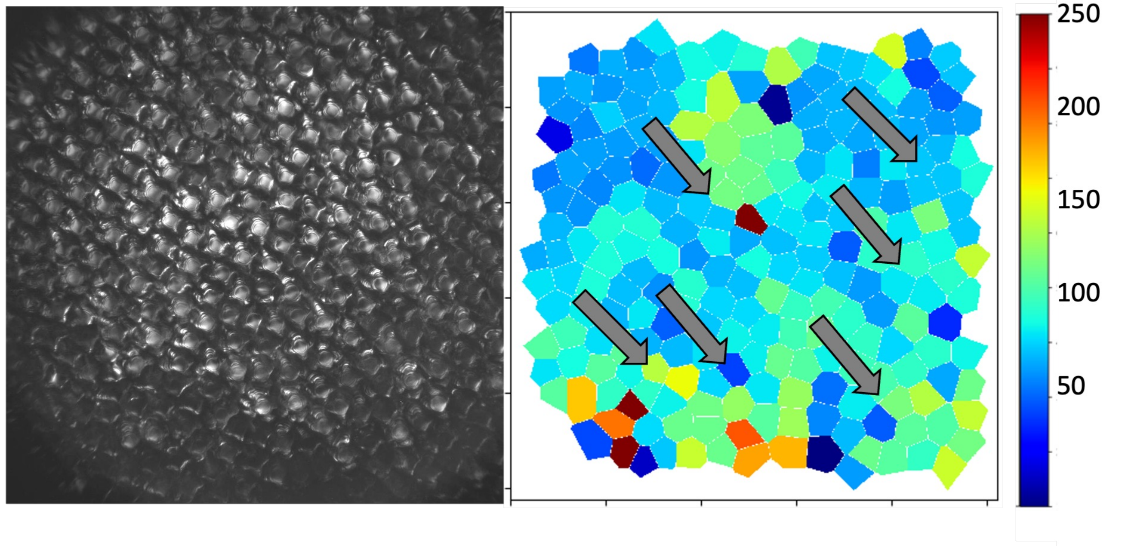
Macroscopic curvature

F. L. Mota et al., Acta Mater. **85**, 362-377 (2015).

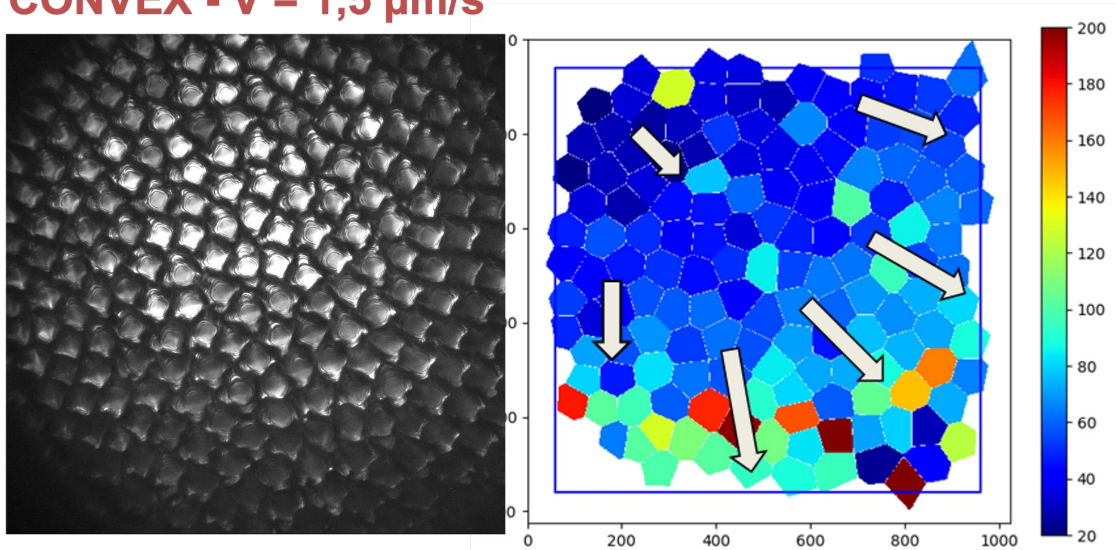
Drifting dynamics – misorientation and curvature

FLAT - V = 3 µm/s

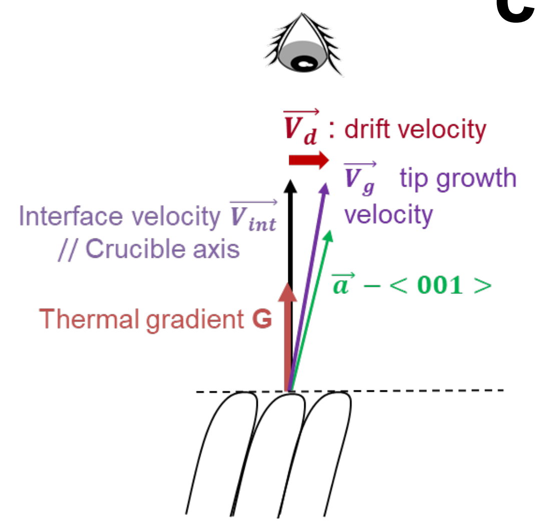
Drift velocity map

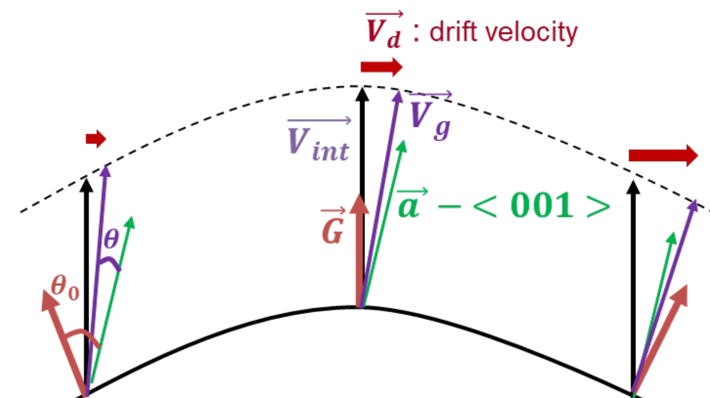


CONVEX - V = 1,5 µm/s



*60 mm of growth, G = 12,5 K/cm ; 7.4*7.4 mm²*





θ_0 : *angle* $(\vec{a}\,;\vec{G})$

θ : *angle* $(\vec{a}\,;\vec{V_g})$

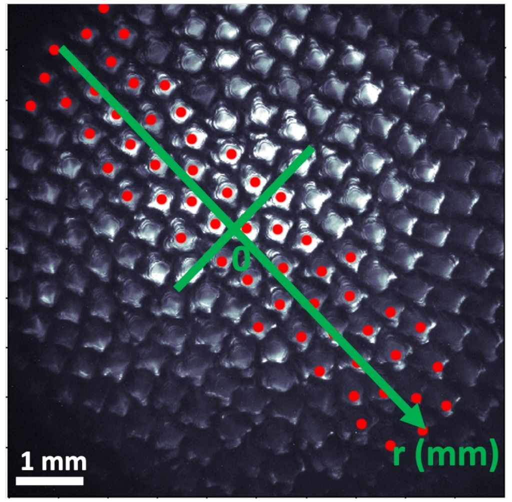
$$\frac{\theta}{\theta_0} = \frac{1}{1 + f\,Pe^g}$$

- Flat interface: Homogeneous drift of the dendritic pattern due to crystallographic misorientation.
- Macroscopic curvature is frequently observed, convex or concave, depending on velocity,
- Curvature modifies radially the misorientation angle => gradient of drift velocity

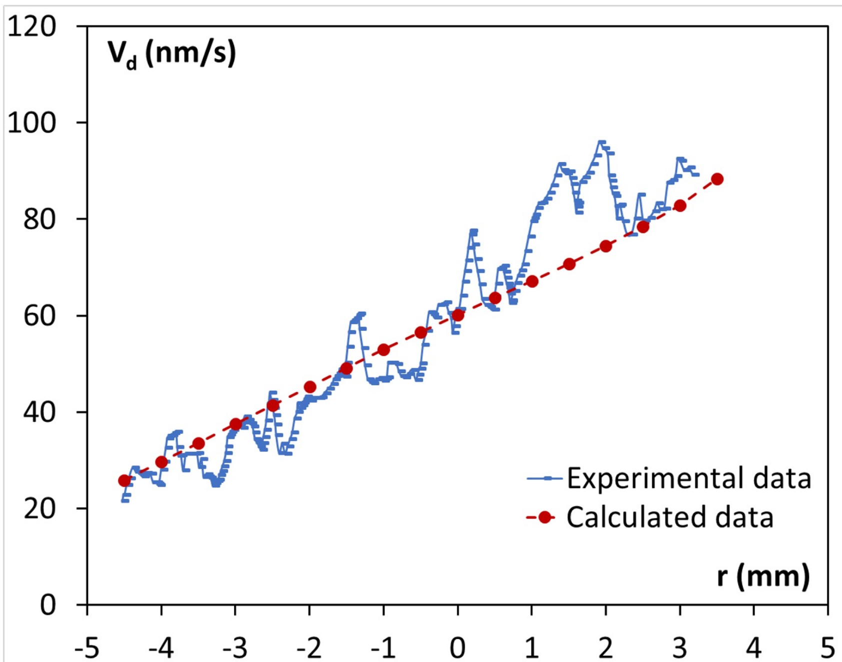
J. Deschamps et al. Phys. Rev. E **78**, 011605 (2008).
S. Akamatsu & T. Ihle, Phys. Rev. E **51,** 4751(1995)

How does the drift velocity profile build ?

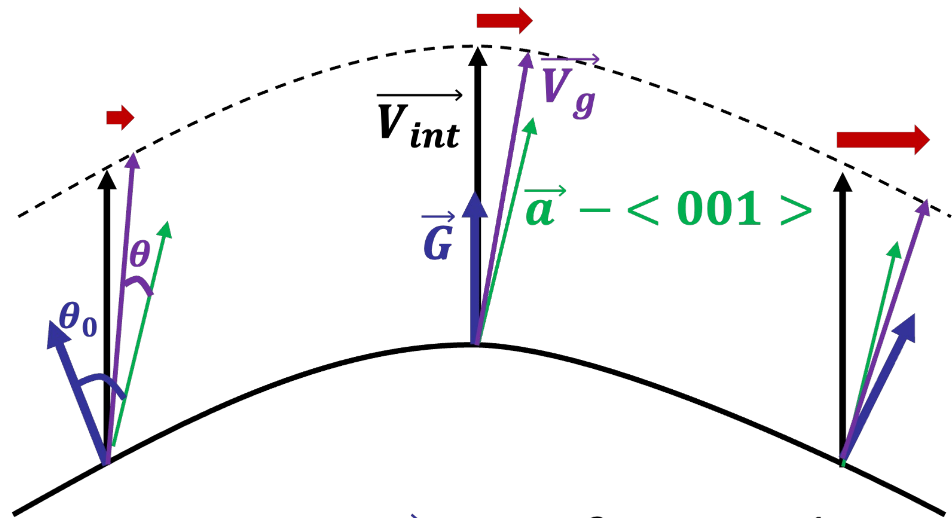
V = 1,5 µm/s



Drift velocity = f(r)



Curvature modifies radially the misorientation between the thermal gradient and the preferred crystallographic direction of growth



θ_0 : angle $(\vec{a}\,;\vec{G})$

θ : angle $(\vec{a}\,;\overrightarrow{V_g})$

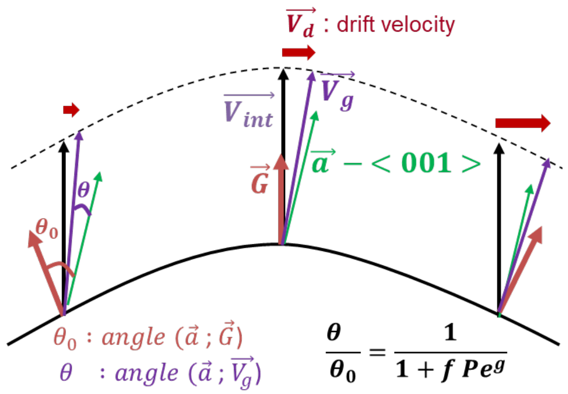
$$\frac{\theta}{\theta_0} = \frac{1}{1 + f\,Pe^g}$$

J. Deschamps et al. Phys. Rev. E **78** (1), 011605 (2008).

Validation of this analysis :

From EXP interface shape, determination of V_drift_calculated as a function of r

➡ **Good agreement with measurements**

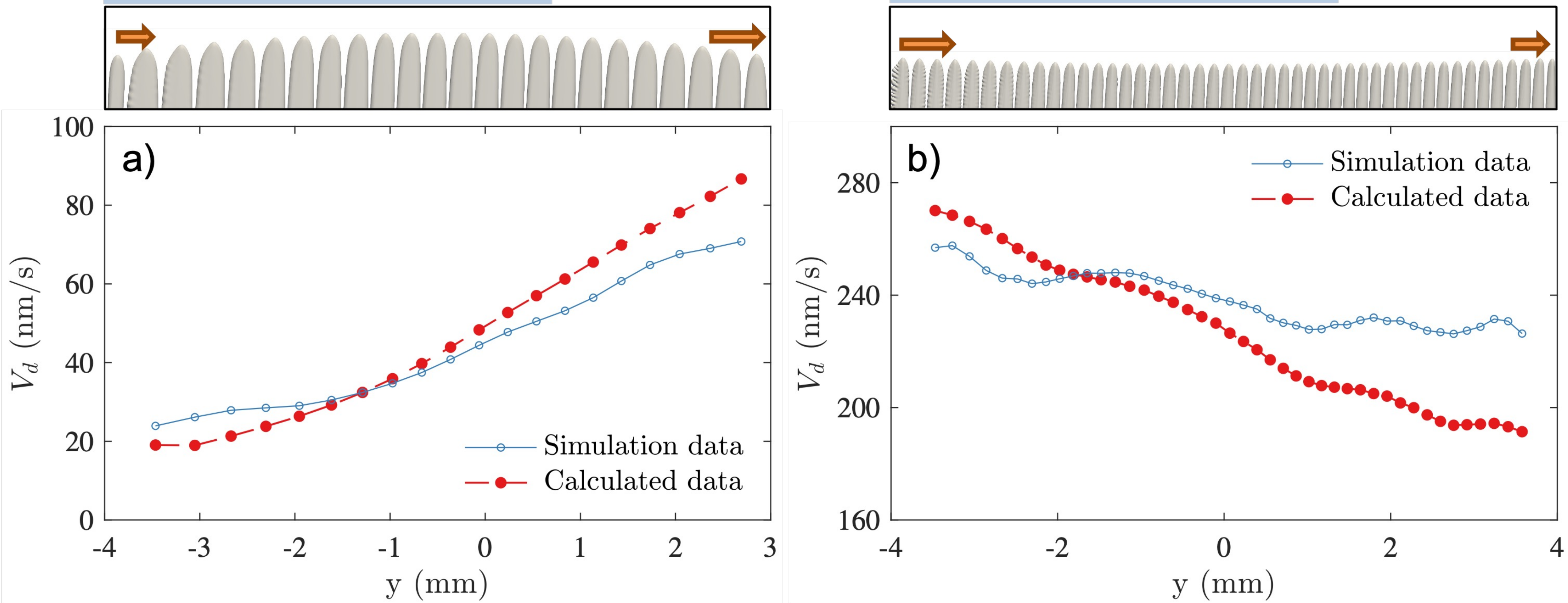


Effect of curvature on drifting velocity

- Velocity gradient: Curvature modifies radially the misorientation angle and causes a gradient of the cell drifting velocity.

V = 1.5 µm/s. Convex interface.

V = 6 µm/s. Concave interface.

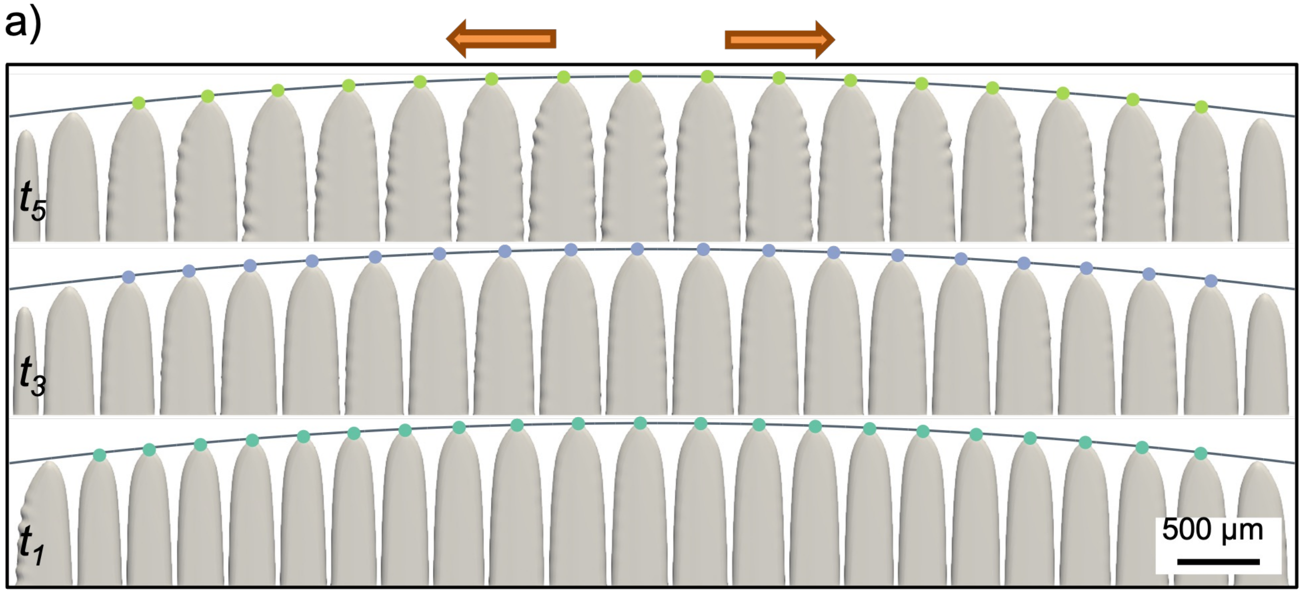


F.L. Mota, K. Ji et al. Acta Mat. (2023): 118849.

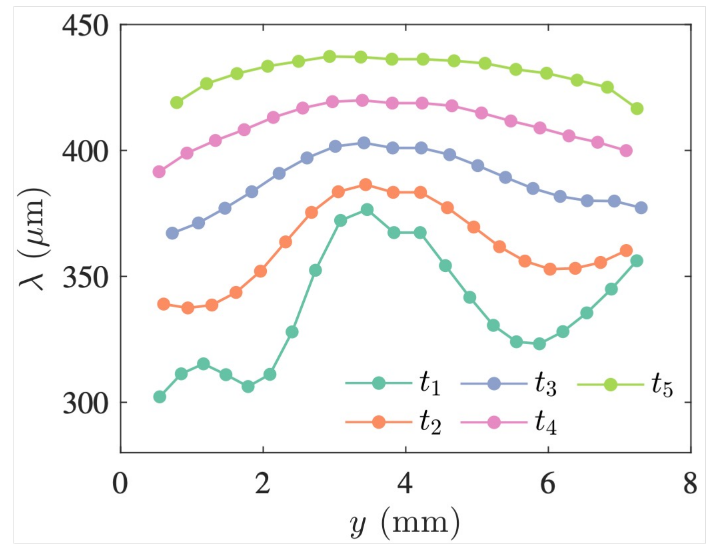
Spacing evolution due to curvature

- Dendrites drift towards the sample boundaries due to a convex curvature and towards the sample center due to a concave curvature. The spacing distribution evolves.

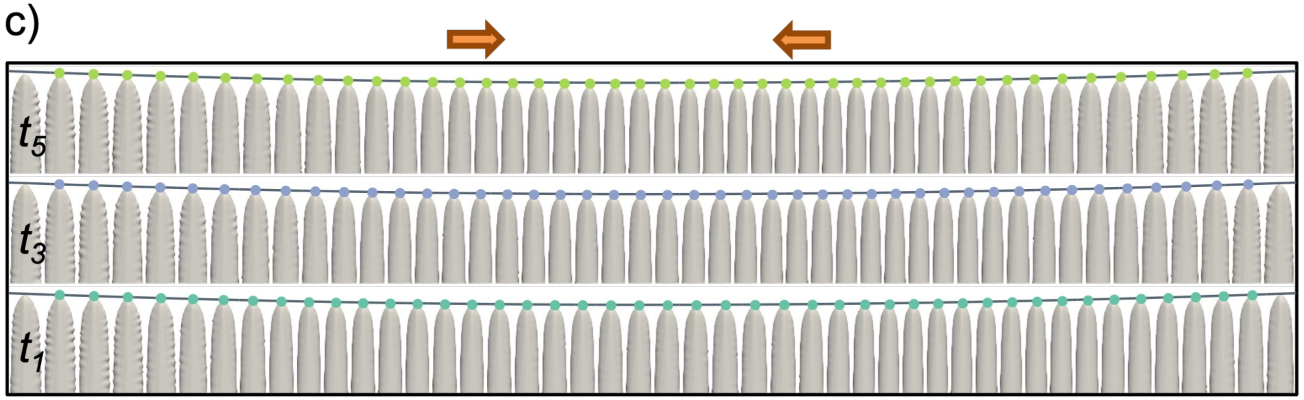
a)



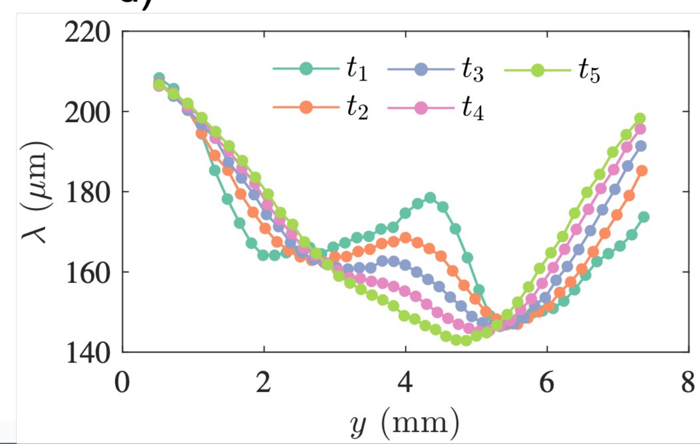
b)



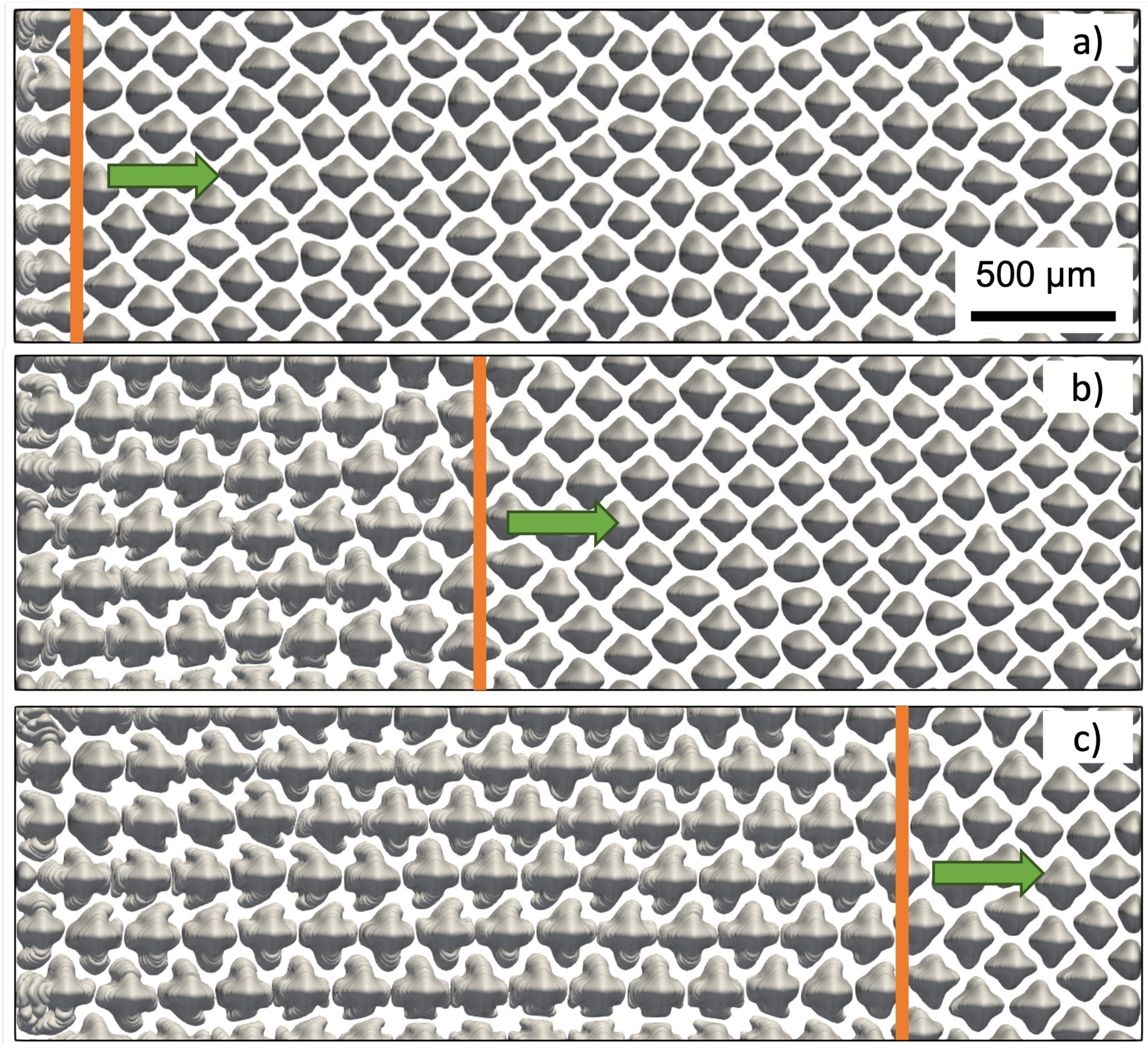
c)



d)

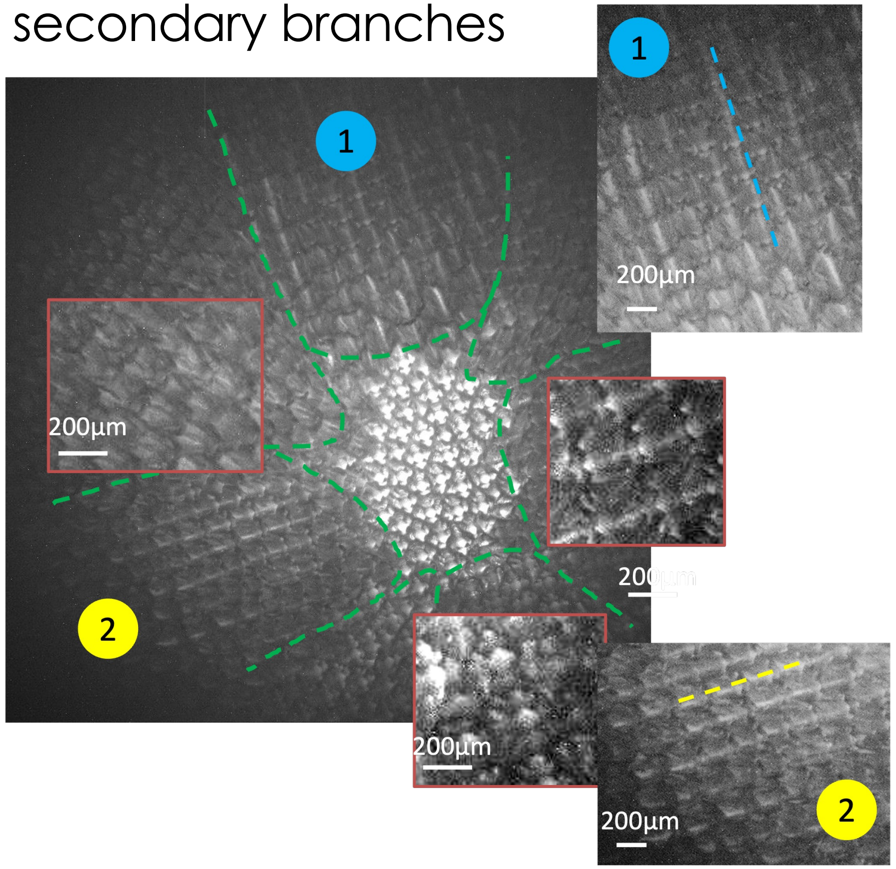


SCN-0.46 wt% camphor alloy, G = 12 K/cm, V = 1.5 (a)-(b) and 6 (c)-(d) µm/s



→ **Stray-grains invasion**
⇒ induces disappearance of the well-oriented grain

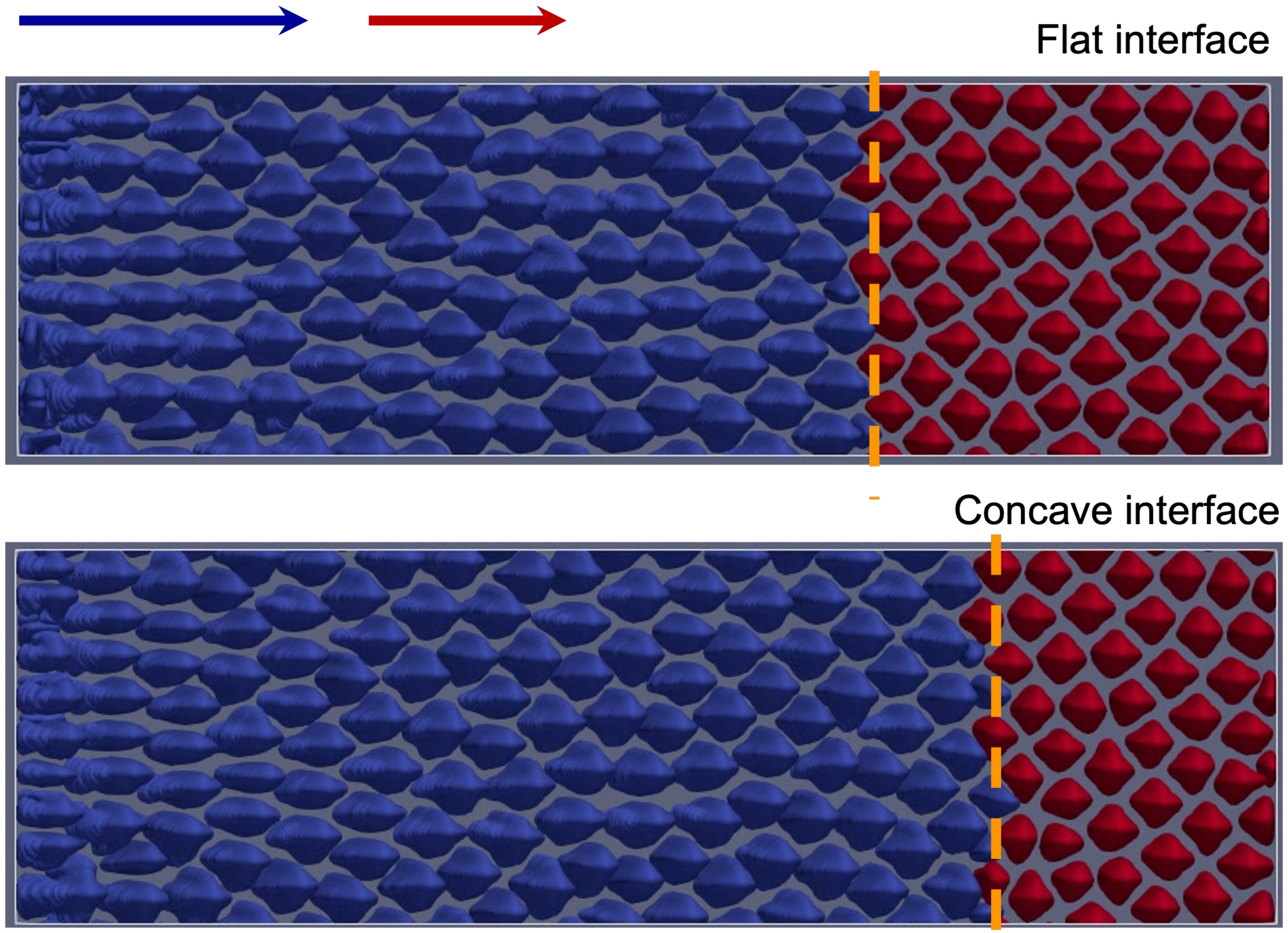
→ **Unusual pattern ordering**
Alignment of dendrites // secondary branches



F.L. Mota, K. Ji et al. Acta Mat. (2023): 118849.

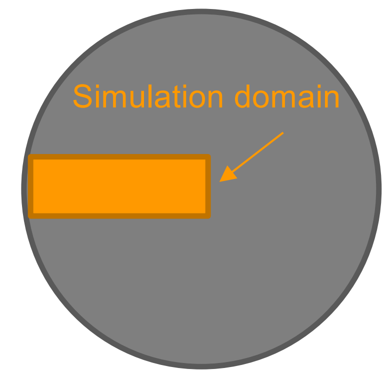
G = 12 K/cm and C_0 = 0.46wt% at V = 6 µm/s

Combined effects of macroscopic curvature and grain boundary



- The migration of a convergent grain boundary under the influence of a macroscopically concave interface.

- The grain boundary migrates faster under a concave interface compared with a flat interface.



*G = 12 K/cm and C_0 = 0.46wt% at V = 6 μm/s; Misorientation **8.1 deg** for the blue grain and **2.7 deg** for the red grain*

Summary

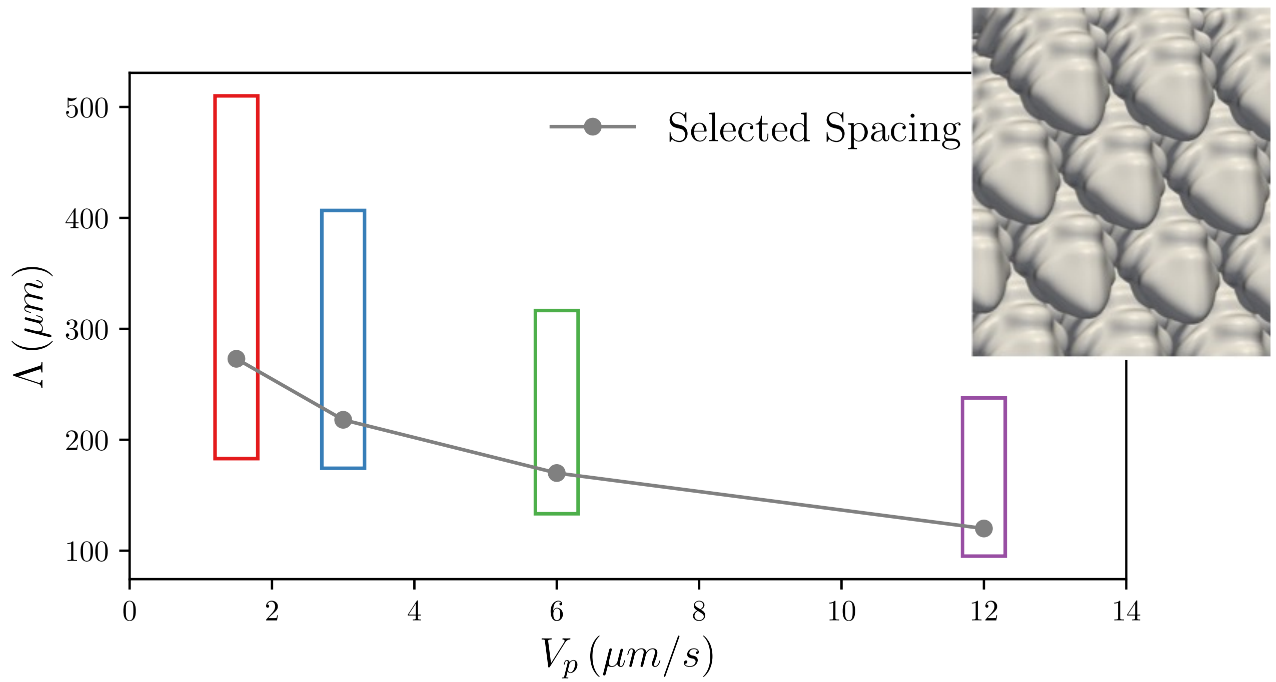
- Observation of dendritic patterns in **DSI-R** experiments and quantitative comparison with 3D phase-field simulations:
  - ➢ From the top view, the morphological instability and interface recoil.
  - ➢ From interferometry, the measurement of tip radius.
  - ➢ From the side view, macroscopic interface curvatures.

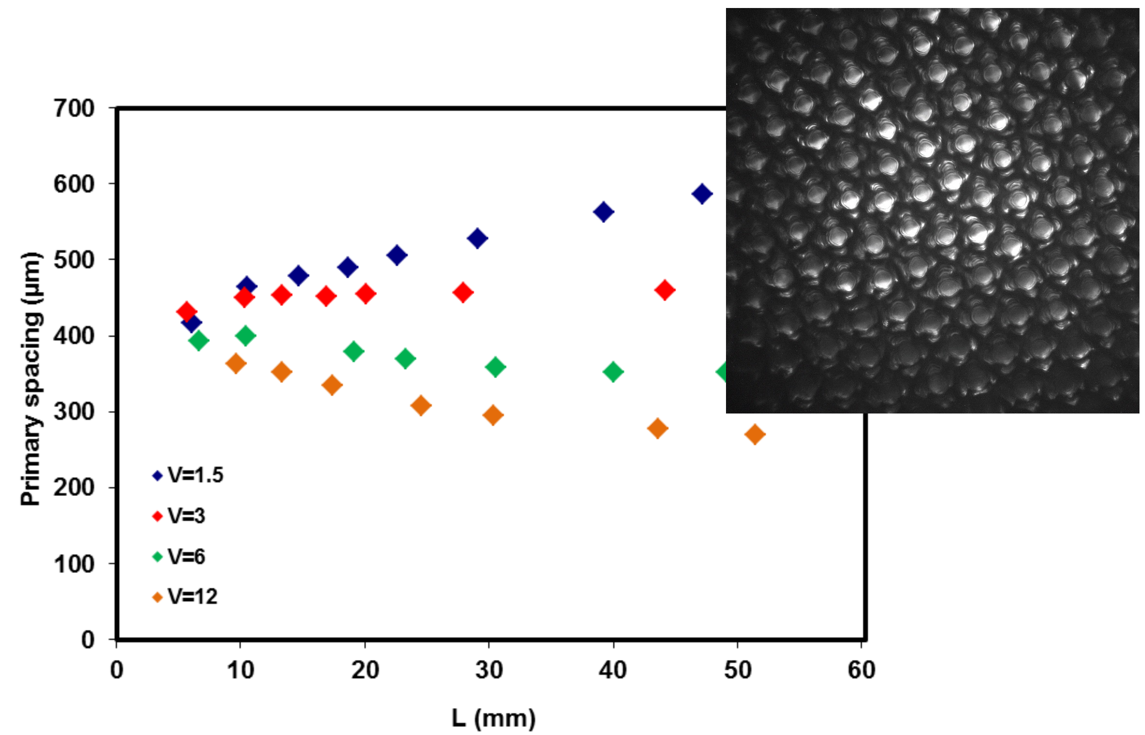
- Even a weak **macroscopic curvature** can create a gradient of lateral drifting velocity and affect the global behavior of growth interfaces.

- Microstructure evolution is affected by the **combined effects** of crystal misorientation, macroscopic curvatures, and grain boundary.

Outlook

- Quantitative comparison between PF simulation and DSI-R experiment.
- Investigate why the upper limit of primary spacing predicted by the phase-field simulation is lower than the experimental observation.
- Investigate the dendrite orientation transition.





Acknowledgement

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Marshall Space Flight Center

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Thank you

for your attention